1983-Pos Board B120
Molecular Identification of the Earthworm Amynthas Gracilis
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Earthworms have been widely used as bio-indicators of soil quality. In such works, the precise identification of the species is a ''sine qua non'' condition. The use of morphological parameters for species identification is difficult and, sometimes just impossible (e.g. identification of juveniles). Intending to investigate the potential use of *Amynthas gracilis* as bio-indicators of soil quality, we first decided to evaluate the molecular identification of *A. gracilis* by means of DNA markers. In order to reach this objective, DNA extractions were performed with specimens acquired from farms of earthworms. The standardization of the method was based on protocols described previously. PCR reactions were performed with the use of two molecular markers: 16S rDNA and *COI*. The chemical conditions of the reactions followed procedures used in the laboratory. The amplification cycles considered annealing temperatures of 44°C for 16S rDNA and 49°C for *COI*. Automatic sequencing was performed on 3500 Genetic Analyzer (Applied Biosystems) and whit BigDye version 3.1 for reactions. Until now, we were able to analyze just five specimens using the BLAST tool of GenBank. For both markers was possible to recovery matches of 100% of identity with *A. gracilis* sequences deposited in the databank, indicating the potential of these markers for molecular identification of this species. However, for both markers we were able to get matches of 98% and 99% of identity with other *A. gracilis* GenBank accessions, and in the case of 16S, 99% of identity with one access of *A. diffringens*. These results may suggest the presence of some intraspecific variability, and for 16S marker, the variability intraspecific and interspecific may be similar in some cases, what, if confirmed, could difficult its application for molecular identification. Further studies will be necessary to clarify these questions.

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Molecular Dynamics Investigations of Z[WC] DNA and the B to Z-DNA Transition
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Although DNA is most commonly found in the right-handed B-DNA structure, it is known that biologically active systems also contain left-handed ZII-DNA. We investigate the possibility that Z[WC]-DNA serves as an intermediate structure in the B to ZII transition. Molecular dynamics simulations indicate that Z[WC] forms stable structures with the current AMBER nucleic acid force field. Steered molecular dynamics simulations indicate that, for collective transitions of the whole strand, the B-Z[WC]-ZII pathway may have a lower free-energy barrier than the direct B-ZII pathway. A careful combination of steered and targeted molecular dynamics, along with umbrella sampling, are used to produce potentials of mean force for both the direct and the B-Z[WC]-ZII pathways.

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Structure and Thermodynamics of Aegis Nucleotides P and Z in DNA
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Artificially expanded genetic information systems (AEGIS) enhance synthetic biology and in vitro primers, probes, and sensors. DNA/RNA design requires the prediction of secondary structures including the expanded alphabet nucleotides. This requires nearest-neighbor thermodynamics analogous to those used for DNA and RNA as well as at least a qualitative understanding of the structure and stability of mismatches. Absorbance melting experiments are presented on oligonucleotides containing P:Z base pairs and P:C, P:T, Z:G, and Z:A mismatches, providing $\Delta\Delta H^\circ$, $\Delta\Delta S^\circ$, and $\Delta\Delta G^\circ_{37}$ values for the modified base pairs. P:Z forms a slightly more stable base pair than G:C, primarily due to entropic stabilization, and the G:Z mismatch is significantly more stable than G:T. Wobble geometries are proposed for the G:Z and P:C mismatches. This work demonstrates that substitution of P for G and Z for T can be a useful tool for the control of the relative thermodynamic stabilities of representative designed secondary structures.

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Binding Studies of Small Molecules to Telomeric Quadruplex DNA for Targeted Singlet Oxygen Production
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Recent studies [*Shieh et al., ACSNano (2010), 4, 1433; Yin et al., Chem. Comm (2012), 48, 6556*] have suggested that G-quadruplexed DNA (qDNA) structures can serve as carriers for targeted delivery of photosensitizers in photodynamic therapies. In our studies, we have investigated the *in vitro* singlet oxygen production from the photosensitive porphyrins, N-methyl mesoporphyrin IX (NMM) and 5,10,15,20-tetrakis(N-methyl-4-pyridyl)-21H,23H-porphine tetratosylate ($TMPyP_4$), when bound to both calf thymus duplex DNA (ct-DNA) and K^+-stabilized G-quadruplexed human $(hTTAGGG)_4$ telomeric DNA (qDNA). Competition micro-dialysis assays confirmed selective binding of NMM to the mixed hybrid qDNA conformation over $TMPyP_4$, which binds non-selectively to both qDNA and ct-DNA. Sensitized singlet oxygen production was detected using the fluorescent singlet oxygen sensor green (SOSG) assay immediately following porphyrin-DNA irradiation. First-order singlet oxygen generation was detected for both NMM and $TMPyP_4$ when bound to qDNA. However, no appreciable singlet oxygen production was detected for NMM when bound to ct-DNA suggesting potential targeted chemotherapeutic applications for NMM bound to qDNA. CD-studies suggest no change in conformation of the qDNA following irradiation. Currently, we are investigating the effect of the Na^+-stabilized antiparallel qDNA conformation on rate and efficiency of singlet oxygen production from these porphyrins. (Supported by NIH-SCORE GM 095437-04.)

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Regulation of the 3' UTR in BDNF mRNA at the DNA Level
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Brain-derived neurotrophic factor (BDNF) is part of the neurotrophic family of genes that encodes for proteins that are known to promote survival of neurons in the peripheral and central nervous systems. The expression of the BDNF gene results in the production of two mRNAs with different lengths, one with a short 3' untranslated region (UTR) and the second with a long 3' -UTR, which are believed to serve different functionalities. The ratio of long to short 3' -UTR in BDNF mRNA changes in different regions of the brain. The long 3' -UTR mRNA is found in both dendrites and soma, whereas the short 3' -UTR is only found in the soma, implying that the BDNF mRNA with the long 3' -UTR is involved in maintaining the neuroplasticity of the brain. Thus, the regulation of the BDNF 3' -UTR length is important, and it may be achieved at the DNA level, at the mRNA level or both. In this study we are investigating the potential of a 20 nucleotide DNA sequence located in the BDNF gene to adopt non-canonical G quadruplex and i-motif structures that might be involved in regulating the production of long versus short length BDNF mRNA 3′-UTR.

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Quantitative Investigation of the Role of SeqA in Escherichia Coli Chromosome Segregation
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Although many bacterial species possess a set of par genes responsible for chromosome segregation, Escherichia coli and a number of other gram-negative bacteria appear to be missing the canonical par genes. Nevertheless, these bacteria do possess a unique set of genes that are found only in species that lack the canonical partitioning system, suggesting that a subset of these genes may have superseded their function. Among this subset is the DNA-binding protein SeqA, already known to play a central role in the regulation of DNA replication. Combining high-throughput fluorescence microscopy and automated image analysis, we are investigating the role of SeqA in segregation by two complementary approaches: (1) characterizing correlated dynamics of SeqA and the origin of replication by simultaneous visualization of SeqA and oriC localization throughout the segregation process in hundreds of independent cells, and (2) quantitative analysis of chromosome dynamics in a SeqA mutant to estimate the magnitude of the biasing forces during the segregation process with and without SeqA. We believe this quantitative imaging-based approach will provide new insights into the segregation process in E. coli which has so far thwarted traditional genetic approaches.